Full wwPDB NMR Structure Validation Report (i)

Apr 21, 2024 – 12:57 AM EDT

PDB ID	:	2L7B
BMRB ID	:	15744
Title	:	NMR Structure of full length apoE3
Authors	:	Chen, J.; Wang, J.
Deposited on	:	2010-12-07

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

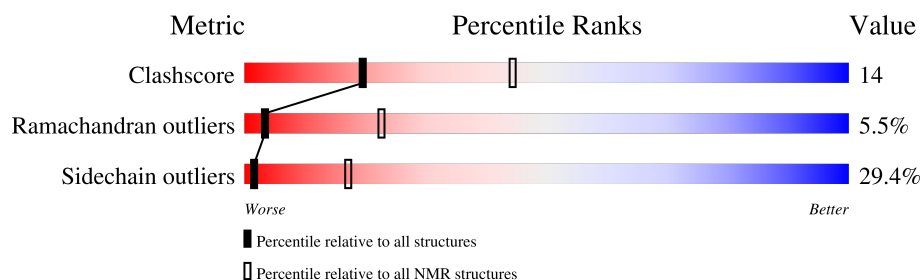|		
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 67%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Clashscore		14
Ramachandran outliers		5.5%
Sidechain outliers		29.4%

Worse   *Better*

▮ Percentile relative to all structures
◨ Percentile relative to all NMR structures

Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	307	47% 40% • 7% •

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 9 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:3-A:181, A:186-A:200, A:209-A:281, A:287-A:296 (277)	0.92	9

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 5 clusters and 3 single-model clusters were found.

Cluster number	Models
1	1, 3, 6, 13, 17
2	7, 10, 11, 20
3	5, 9, 19
4	12, 14, 15
5	2, 4
Single-model clusters	8; 16; 18

3 Entity composition ⓘ

There is only 1 type of molecule in this entry. The entry contains 4792 atoms, of which 2396 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Apolipoprotein E.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	299	4792	1464	2396	459	465	8	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	HIS	-	expression tag	UNP P02649
A	-6	HIS	-	expression tag	UNP P02649
A	-5	HIS	-	expression tag	UNP P02649
A	-4	HIS	-	expression tag	UNP P02649
A	-3	HIS	-	expression tag	UNP P02649
A	-2	HIS	-	expression tag	UNP P02649
A	-1	HIS	-	expression tag	UNP P02649
A	0	HIS	-	expression tag	UNP P02649
A	257	ALA	PHE	engineered mutation	UNP P02649
A	264	ARG	TRP	engineered mutation	UNP P02649
A	269	ALA	VAL	engineered mutation	UNP P02649
A	279	GLN	LEU	engineered mutation	UNP P02649
A	287	GLU	VAL	engineered mutation	UNP P02649

4 Residue-property plots ⓘ

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.
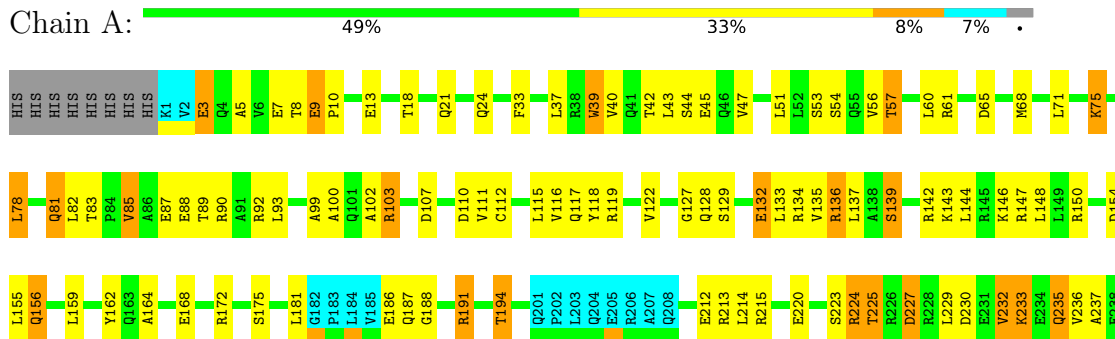
• Molecule 1: Apolipoprotein E
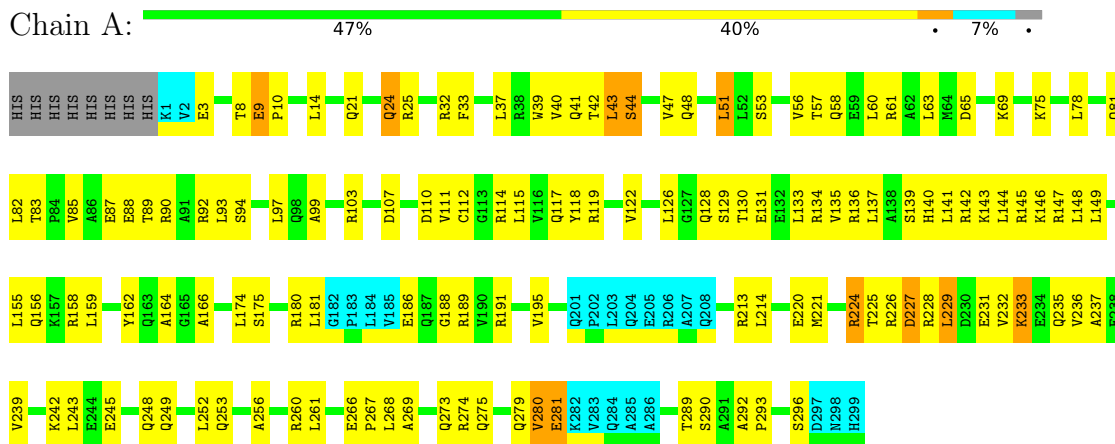
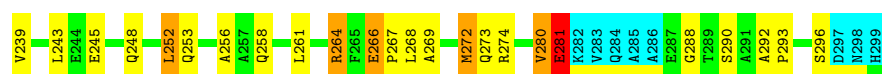## 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Apolipoprotein E

4.2.2 Score per residue for model 2

• Molecule 1: Apolipoprotein E

Chain A:

4.2.3 Score per residue for model 3

• Molecule 1: Apolipoprotein E

Chain A:

4.2.4 Score per residue for model 4

• Molecule 1: Apolipoprotein E

Chain A:

4.2.5 Score per residue for model 5

● Molecule 1: Apolipoprotein E

4.2.6 Score per residue for model 6

● Molecule 1: Apolipoprotein E
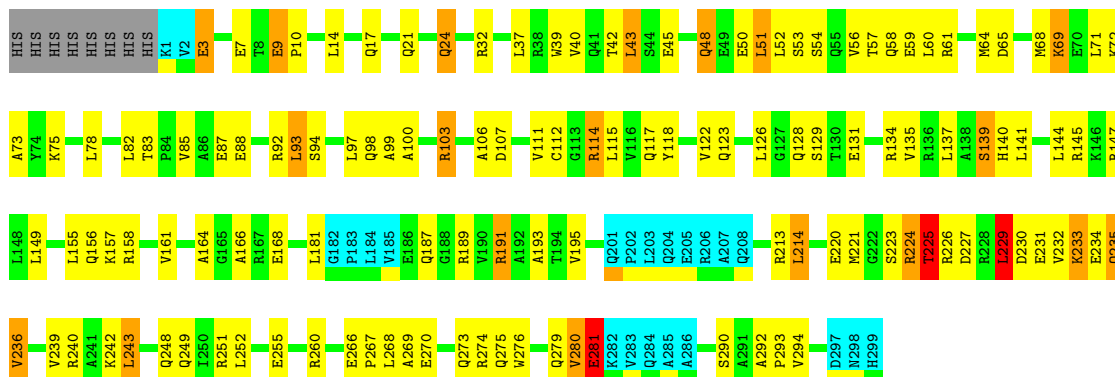
4.2.7 Score per residue for model 7
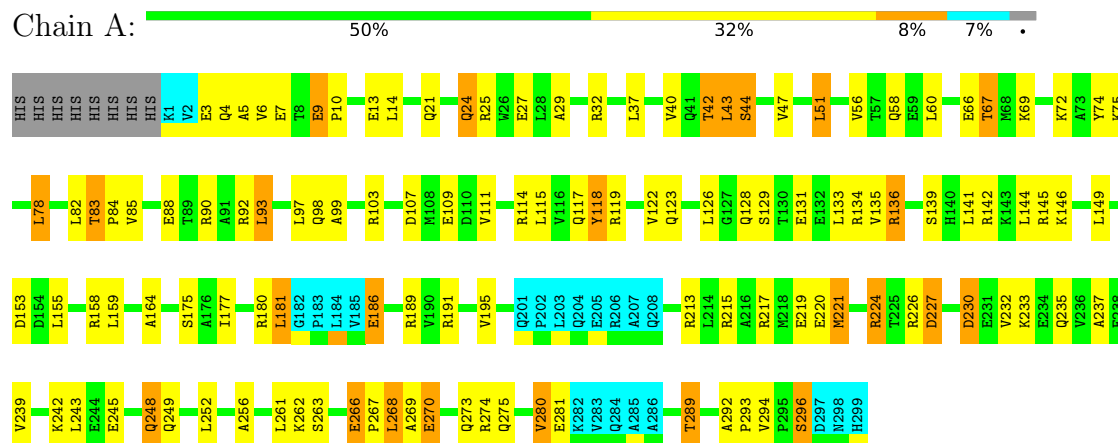
• Molecule 1: Apolipoprotein E

4.2.8 Score per residue for model 8

• Molecule 1: Apolipoprotein E

4.2.9 Score per residue for model 9 (medoid)
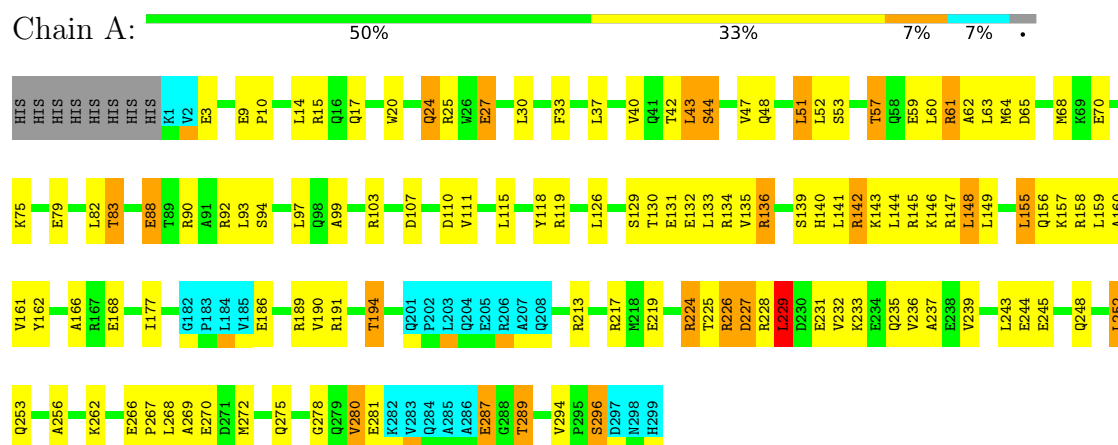
• Molecule 1: Apolipoprotein E
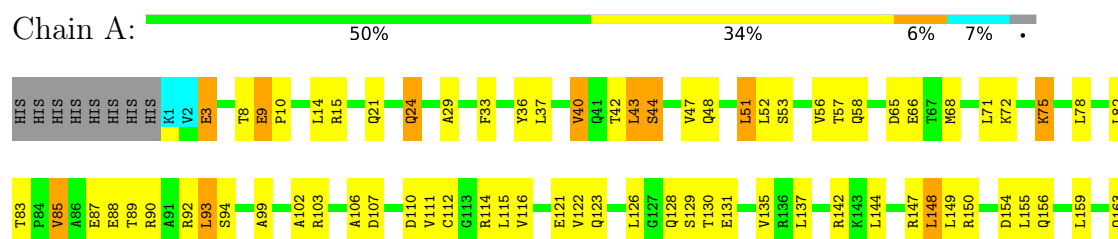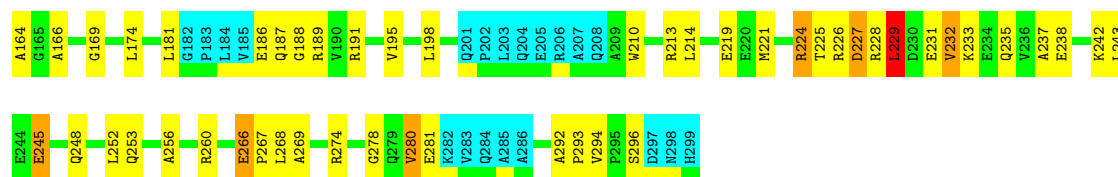
4.2.10 Score per residue for model 10

● Molecule 1: Apolipoprotein E

Chain A:
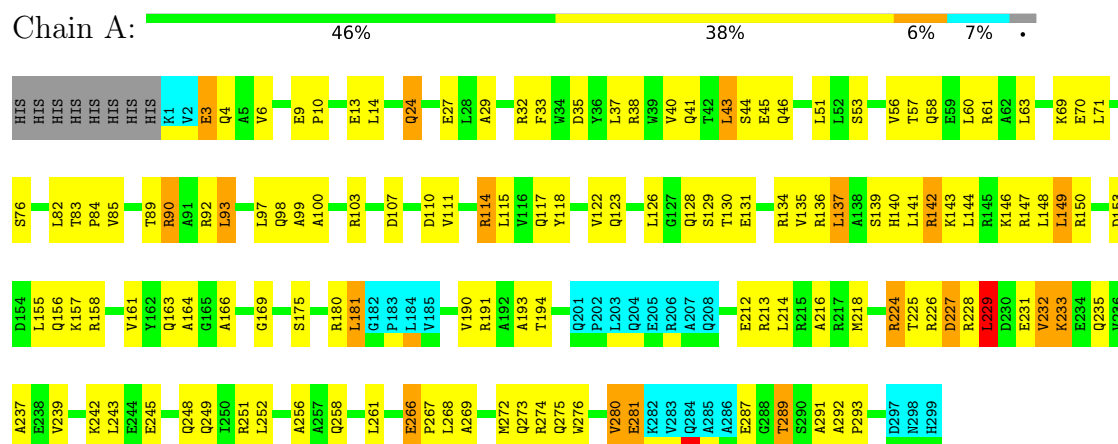
4.2.11 Score per residue for model 11

● Molecule 1: Apolipoprotein E

Chain A:
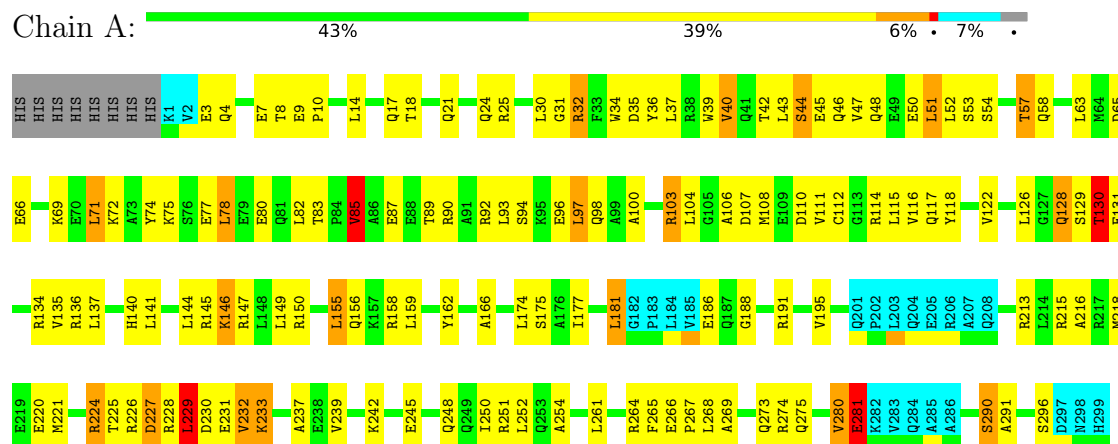
4.2.12 Score per residue for model 12

● Molecule 1: Apolipoprotein E

Chain A:
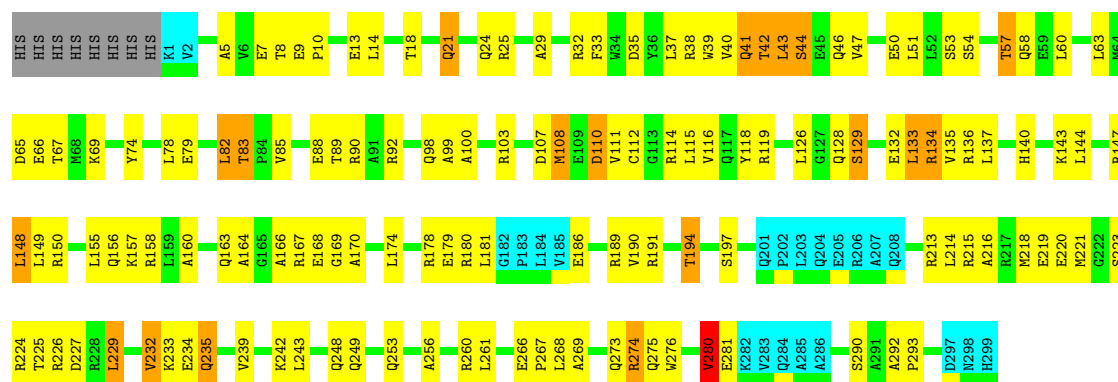
4.2.13 Score per residue for model 13
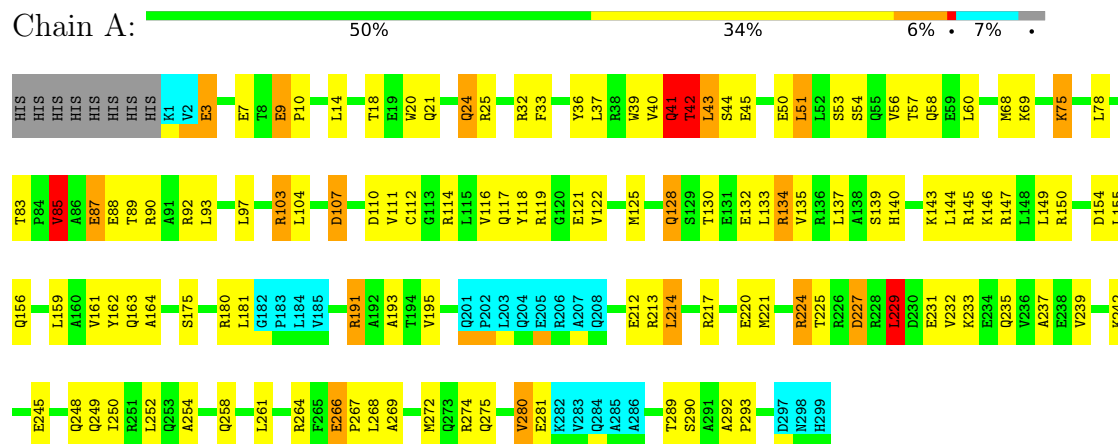
• Molecule 1: Apolipoprotein E
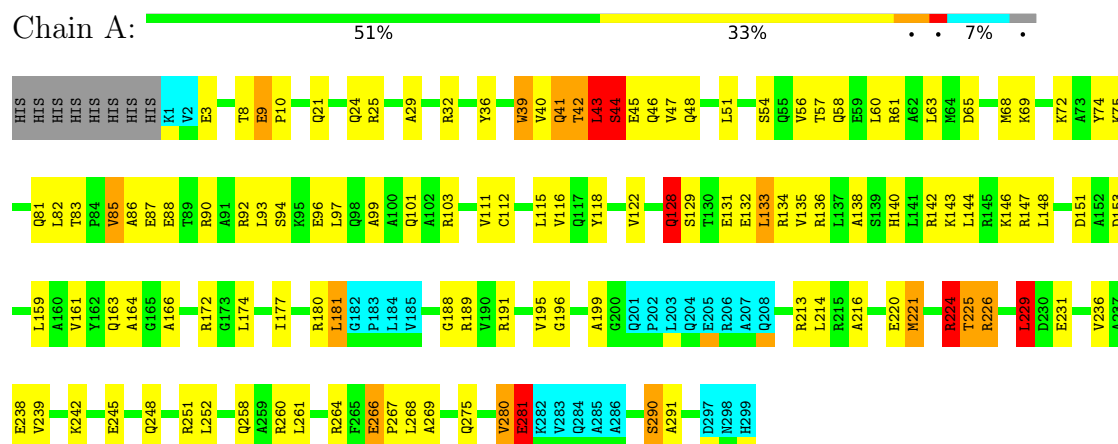
4.2.14 Score per residue for model 14

• Molecule 1: Apolipoprotein E
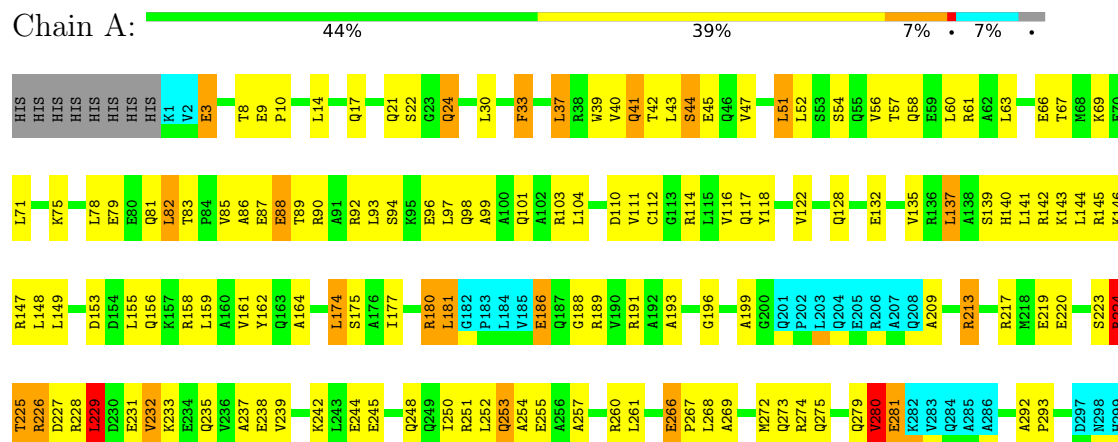
4.2.15 Score per residue for model 15

• Molecule 1: Apolipoprotein E
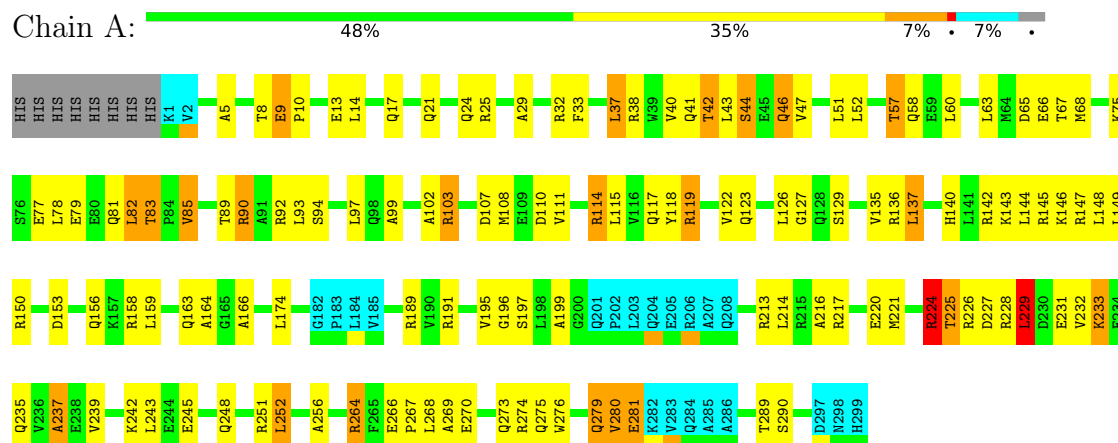
4.2.16 Score per residue for model 16
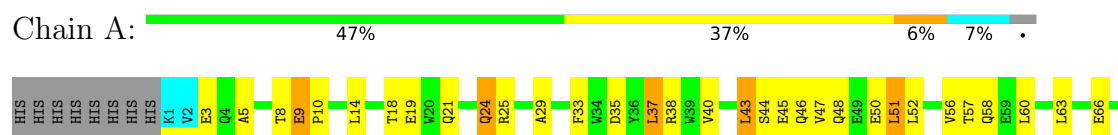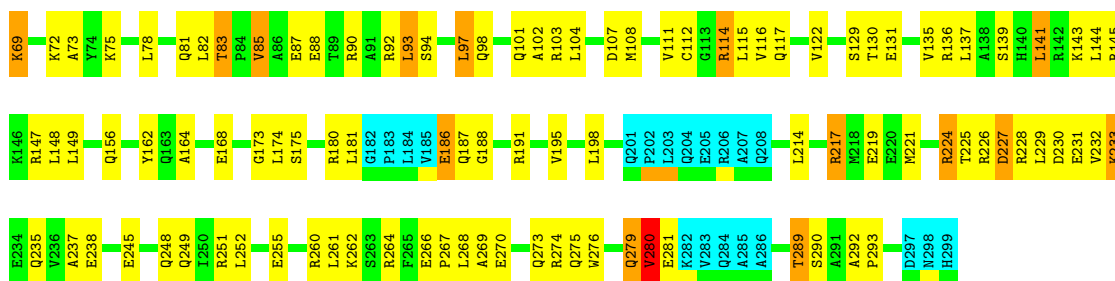
• Molecule 1: Apolipoprotein E
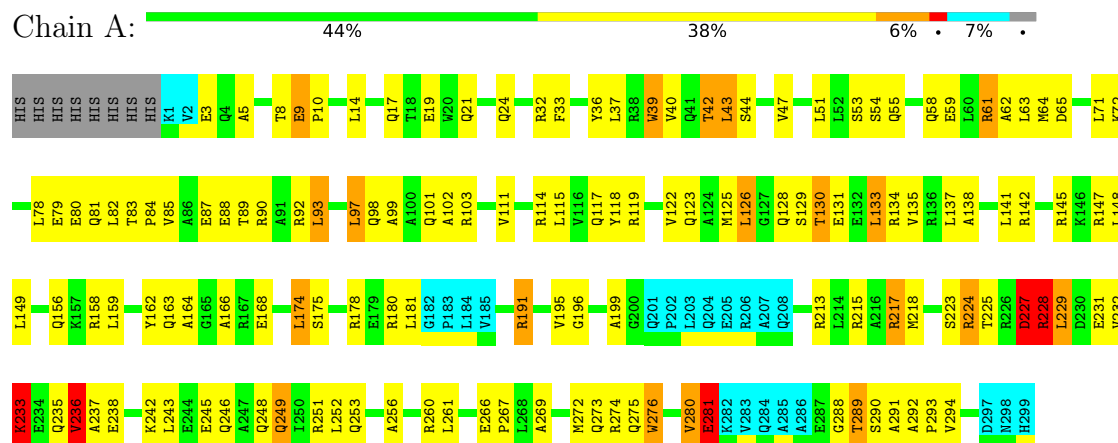
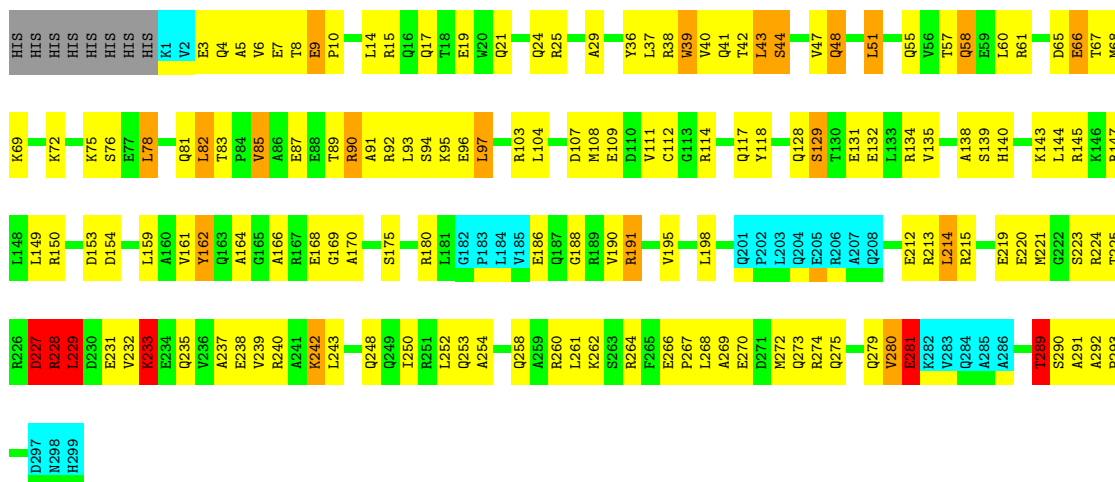### 4.2.17 Score per residue for model 17

• Molecule 1: Apolipoprotein E
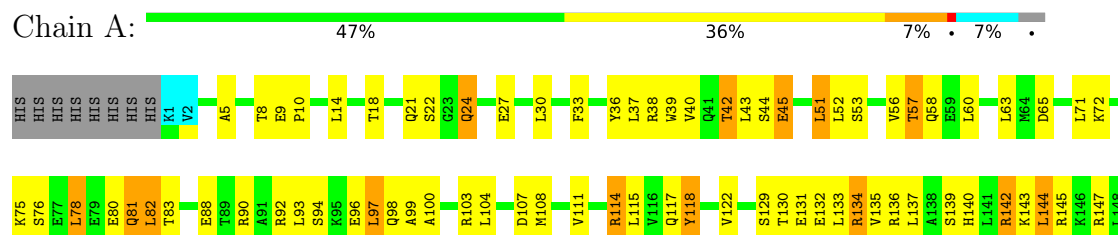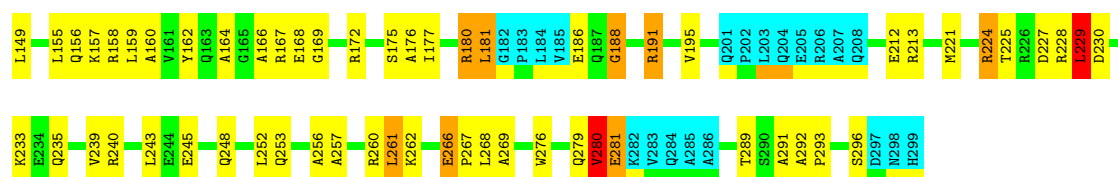
4.2.18 Score per residue for model 18

● Molecule 1: Apolipoprotein E

Chain A:
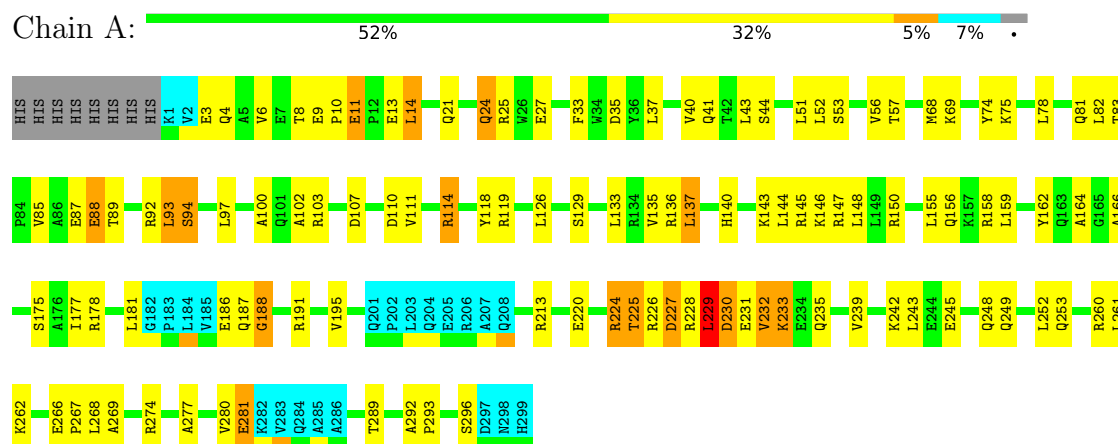
4.2.19 Score per residue for model 19

● Molecule 1: Apolipoprotein E

Chain A:
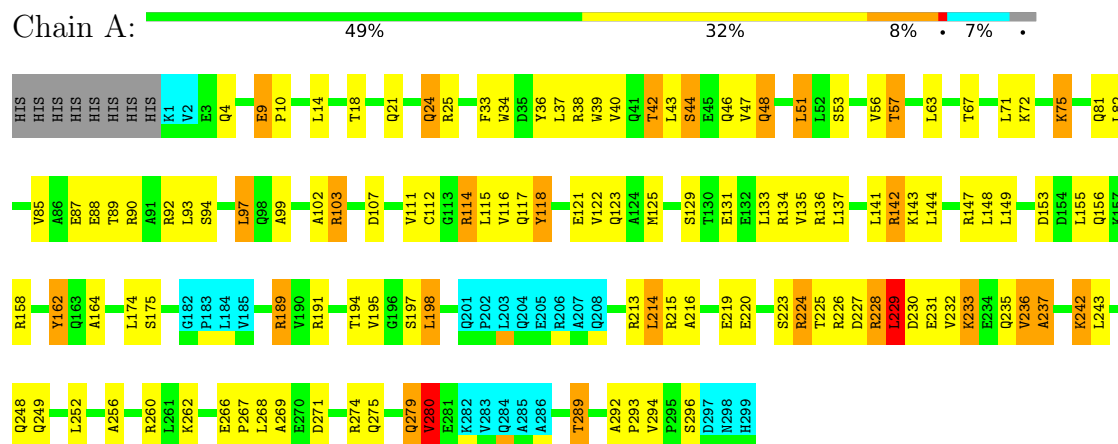
4.2.20 Score per residue for model 20

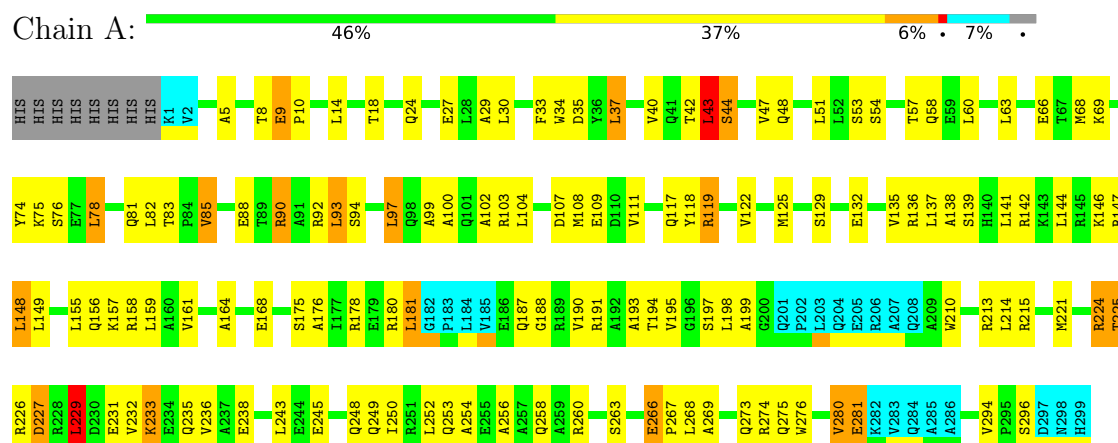● Molecule 1: Apolipoprotein E

Chain A:

HIS HIS HIS HIS HIS HIS HIS HIS K1 V2 E7 T8 E9 P10 L14 R15 T18 Q24 R32 F33 W34 L37 R38 W39 V40 Q41 T42 L43 S44 E45 Q46 V47 Q48 L51 S54 T57 Q58 R61 D65 K75 L78 Q81 L82 T83 P84 V85

A86 E87 E88 T89 R92 L93 S94 K95 E96 L97 Q98 A99 R103 D107 V111 C112 L115 V116 Q117 Y118 V122 M125 L126 G127 Q128 E131 E132 L133 R134 V135 R136 L137 A138 S139 H140 L141 R142 K143 L144 R145 K146 R147 L148 L149 R150 Q156 L159 Y162

A166 R167 E168 G169 A170 E171 S175 A176 I177 R178 E179 R180 L181 G182 P183 L184 V185 E186 Q187 G188 R189 V190 R191 A192 A193 T194 Q201 P202 L203 Q204 E205 R206 A207 Q208 A209 W210 R213 L214 R215 A216 M221 R224 T225 R226 D227 R228 L229 V232 K233 E234 Q235 V236 A237 E238

V239 K242 E245 Q248 L252 A256 A257 Q258 A259 R260 L261 F265 E266 P267 L268 A269 M272 Q273 R274 Q275 Q279 V280 E281 K282 V283 Q284 A285 A286 S290 A291 A292 S296 D297 N298 H299

5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *simulated annealing, distance geometry.*

Of the 20 calculated structures, 20 were deposited, based on the following criterion: *all calculated structures submitted.*

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
CYANA	structure solution	
ProcheckNMR	geometry optimization	
ProcheckNMR	refinement	
CNS	geometry optimization	
CNS	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	2810
Number of shifts mapped to atoms	2810
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	67%

6 Model quality ⓘ

6.1 Standard geometry ⓘ

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	2226	2221	2221	62±7
All	All	44520	44420	44420	1248

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:78:LEU:HD13	1:A:159:LEU:HD22	0.99	1.35	2	2
1:A:51:LEU:HD13	1:A:122:VAL:HG11	0.96	1.35	2	4
1:A:111:VAL:HG22	1:A:144:LEU:HD21	0.95	1.34	7	13
1:A:243:LEU:HD23	1:A:294:VAL:HG22	0.93	1.35	16	1
1:A:243:LEU:HD21	1:A:294:VAL:HG23	0.86	1.48	9	3
1:A:43:LEU:HD12	1:A:137:LEU:HD21	0.83	1.49	20	2
1:A:71:LEU:HD22	1:A:104:LEU:HD23	0.82	1.50	11	1
1:A:82:LEU:HD13	1:A:93:LEU:HD22	0.81	1.51	10	2
1:A:82:LEU:HD13	1:A:93:LEU:HD21	0.79	1.52	9	2
1:A:51:LEU:HD21	1:A:122:VAL:HG11	0.75	1.59	4	1
1:A:14:LEU:HD22	1:A:149:LEU:HD21	0.74	1.60	14	9
1:A:149:LEU:HD23	1:A:280:VAL:HG12	0.73	1.58	4	3
1:A:43:LEU:HD22	1:A:47:VAL:HG23	0.71	1.61	20	2
1:A:78:LEU:HD22	1:A:159:LEU:HD23	0.71	1.62	20	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:82:LEU:HD21	1:A:93:LEU:HD13	0.70	1.64	4	1
1:A:51:LEU:HD11	1:A:118:TYR:CE2	0.70	2.21	15	6
1:A:268:LEU:O	1:A:269:ALA:HB3	0.69	1.87	20	1
1:A:99:ALA:HB1	1:A:256:ALA:HB2	0.69	1.64	15	6
1:A:100:ALA:HB1	1:A:155:LEU:HD12	0.69	1.63	12	5
1:A:40:VAL:HG11	1:A:141:LEU:HD11	0.69	1.63	11	5
1:A:83:THR:HG22	1:A:161:VAL:HG12	0.68	1.65	3	5
1:A:51:LEU:HD21	1:A:118:TYR:CE2	0.68	2.23	1	7
1:A:40:VAL:HG22	1:A:56:VAL:HG12	0.68	1.63	17	1
1:A:51:LEU:HD21	1:A:118:TYR:CD2	0.68	2.24	11	5
1:A:42:THR:HG22	1:A:217:ARG:HD3	0.67	1.67	14	2
1:A:46:GLN:HG3	1:A:216:ALA:HB3	0.67	1.65	13	4
1:A:33:PHE:CE2	1:A:37:LEU:HD22	0.67	2.24	16	3
1:A:81:GLN:O	1:A:82:LEU:HD13	0.67	1.90	15	3
1:A:131:GLU:O	1:A:135:VAL:HG13	0.66	1.90	13	3
1:A:51:LEU:HD11	1:A:118:TYR:CZ	0.66	2.25	10	7
1:A:85:VAL:HG11	1:A:89:THR:HG21	0.66	1.66	3	3
1:A:140:HIS:CE1	1:A:239:VAL:HG23	0.66	2.26	5	3
1:A:135:VAL:HG21	1:A:232:VAL:CG2	0.66	2.21	20	11
1:A:239:VAL:HG12	1:A:243:LEU:HD22	0.65	1.66	12	3
1:A:33:PHE:CZ	1:A:148:LEU:HD13	0.65	2.27	20	2
1:A:82:LEU:HD12	1:A:93:LEU:HD13	0.65	1.67	8	1
1:A:36:TYR:O	1:A:40:VAL:HG23	0.65	1.92	13	3
1:A:8:THR:HG21	1:A:280:VAL:HG12	0.65	1.68	20	1
1:A:36:TYR:CD2	1:A:63:LEU:HD11	0.65	2.27	19	1
1:A:40:VAL:HG21	1:A:60:LEU:HD11	0.64	1.69	5	3
1:A:43:LEU:HD11	1:A:226:ARG:HB3	0.64	1.68	8	1
1:A:33:PHE:CZ	1:A:37:LEU:HD22	0.64	2.27	20	1
1:A:131:GLU:O	1:A:135:VAL:HG23	0.64	1.91	9	10
1:A:8:THR:HG22	1:A:280:VAL:HG23	0.64	1.68	11	3
1:A:82:LEU:HD12	1:A:93:LEU:HD23	0.64	1.69	11	1
1:A:3:GLU:O	1:A:6:VAL:HG12	0.64	1.92	5	1
1:A:90:ARG:HA	1:A:93:LEU:HD23	0.64	1.69	7	1
1:A:33:PHE:HB2	1:A:63:LEU:HD11	0.64	1.70	12	1
1:A:93:LEU:HD13	1:A:162:TYR:CZ	0.64	2.27	17	1
1:A:37:LEU:O	1:A:40:VAL:HG12	0.64	1.93	15	16
1:A:81:GLN:O	1:A:82:LEU:HD23	0.64	1.93	1	6
1:A:48:GLN:HA	1:A:51:LEU:HD23	0.64	1.70	5	5
1:A:181:LEU:HD11	1:A:186:GLU:OE1	0.63	1.93	11	1
1:A:8:THR:HG21	1:A:149:LEU:CD2	0.63	2.23	14	4
1:A:140:HIS:CE1	1:A:239:VAL:HG13	0.63	2.29	10	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:PHE:CZ	1:A:148:LEU:HD22	0.63	2.29	12	1
1:A:102:ALA:HB3	1:A:252:LEU:HD21	0.63	1.69	1	3
1:A:79:GLU:OE2	1:A:174:LEU:HD12	0.63	1.94	12	3
1:A:43:LEU:HD13	1:A:221:MET:CB	0.63	2.23	13	1
1:A:51:LEU:HD13	1:A:122:VAL:HG21	0.63	1.70	1	6
1:A:82:LEU:HD21	1:A:170:ALA:HA	0.63	1.71	5	3
1:A:27:GLU:OE1	1:A:30:LEU:HD11	0.63	1.94	17	1
1:A:107:ASP:O	1:A:111:VAL:HG23	0.62	1.94	17	15
1:A:3:GLU:OE2	1:A:289:THR:HG23	0.62	1.94	3	3
1:A:248:GLN:OE1	1:A:252:LEU:HD11	0.62	1.95	6	7
1:A:42:THR:HG22	1:A:221:MET:CG	0.62	2.24	11	4
1:A:93:LEU:HD12	1:A:162:TYR:CE1	0.62	2.30	18	1
1:A:83:THR:HG22	1:A:161:VAL:CG1	0.62	2.25	10	6
1:A:139:SER:OG	1:A:229:LEU:HD13	0.62	1.94	6	2
1:A:78:LEU:HD12	1:A:162:TYR:HB2	0.62	1.72	1	1
1:A:268:LEU:O	1:A:269:ALA:CB	0.62	2.48	20	1
1:A:85:VAL:HG11	1:A:89:THR:HG22	0.61	1.71	19	3
1:A:42:THR:C	1:A:43:LEU:HD22	0.61	2.15	19	1
1:A:133:LEU:HD23	1:A:235:GLN:CG	0.61	2.25	1	1
1:A:42:THR:HG22	1:A:221:MET:HG2	0.61	1.71	7	2
1:A:83:THR:O	1:A:166:ALA:HB2	0.61	1.95	11	11
1:A:40:VAL:HG23	1:A:56:VAL:HB	0.61	1.70	14	2
1:A:46:GLN:CG	1:A:216:ALA:HB3	0.61	2.25	11	6
1:A:280:VAL:HG22	1:A:281:GLU:HG3	0.61	1.73	18	5
1:A:82:LEU:HD21	1:A:169:GLY:C	0.61	2.16	10	1
1:A:138:ALA:HB3	1:A:228:ARG:O	0.60	1.96	16	2
1:A:142:ARG:CZ	1:A:229:LEU:HD11	0.60	2.25	1	3
1:A:43:LEU:HD22	1:A:47:VAL:CG2	0.60	2.27	11	1
1:A:74:TYR:CD2	1:A:159:LEU:HD11	0.60	2.32	13	1
1:A:114:ARG:NH2	1:A:137:LEU:HD12	0.60	2.11	6	4
1:A:191:ARG:O	1:A:195:VAL:HG23	0.60	1.96	15	13
1:A:132:GLU:O	1:A:135:VAL:HG22	0.60	1.97	13	5
1:A:264:ARG:NH1	1:A:268:LEU:HD21	0.60	2.12	5	4
1:A:266:GLU:HB2	1:A:267:PRO:HD3	0.60	1.72	6	9
1:A:135:VAL:HG21	1:A:232:VAL:HG21	0.60	1.74	19	6
1:A:33:PHE:HA	1:A:63:LEU:HD23	0.60	1.74	16	2
1:A:112:CYS:O	1:A:116:VAL:HG23	0.60	1.97	3	9
1:A:139:SER:HB2	1:A:229:LEU:HD23	0.59	1.74	8	2
1:A:82:LEU:CD1	1:A:93:LEU:HD23	0.59	2.26	11	1
1:A:117:GLN:NE2	1:A:237:ALA:HB1	0.59	2.12	15	1
1:A:75:LYS:HD2	1:A:159:LEU:HD11	0.59	1.74	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:135:VAL:HG21	1:A:232:VAL:HB	0.59	1.73	12	2
1:A:111:VAL:CG2	1:A:144:LEU:HD21	0.59	2.25	4	7
1:A:37:LEU:HD11	1:A:145:ARG:HG2	0.59	1.74	11	7
1:A:111:VAL:O	1:A:115:LEU:HD23	0.59	1.97	13	6
1:A:40:VAL:HG23	1:A:56:VAL:CG2	0.59	2.26	18	2
1:A:60:LEU:HD13	1:A:111:VAL:CG1	0.59	2.28	14	8
1:A:82:LEU:HD22	1:A:93:LEU:HD13	0.59	1.74	2	1
1:A:8:THR:CG2	1:A:280:VAL:HG12	0.59	2.28	20	1
1:A:60:LEU:HD22	1:A:111:VAL:HG11	0.59	1.71	2	5
1:A:5:ALA:O	1:A:8:THR:HG22	0.59	1.97	12	5
1:A:42:THR:HG23	1:A:217:ARG:HG3	0.59	1.73	3	1
1:A:82:LEU:CD2	1:A:93:LEU:HD13	0.59	2.26	4	1
1:A:46:GLN:HG2	1:A:216:ALA:HB3	0.59	1.74	15	2
1:A:82:LEU:HD22	1:A:162:TYR:CZ	0.59	2.33	19	1
1:A:43:LEU:HD11	1:A:137:LEU:HD22	0.59	1.75	9	1
1:A:81:GLN:C	1:A:82:LEU:HD22	0.59	2.18	13	1
1:A:243:LEU:HD23	1:A:296:SER:HA	0.59	1.75	19	2
1:A:44:SER:O	1:A:47:VAL:HG12	0.58	1.98	15	15
1:A:82:LEU:HD13	1:A:93:LEU:CD2	0.58	2.26	9	4
1:A:43:LEU:HD12	1:A:137:LEU:CD2	0.58	2.24	20	1
1:A:82:LEU:HD22	1:A:93:LEU:CD1	0.58	2.28	1	2
1:A:267:PRO:HG2	1:A:268:LEU:HD23	0.58	1.75	11	15
1:A:82:LEU:CD2	1:A:166:ALA:HB3	0.58	2.27	11	2
1:A:280:VAL:HG12	1:A:281:GLU:HG3	0.58	1.75	16	2
1:A:75:LYS:HA	1:A:78:LEU:HD23	0.58	1.74	11	1
1:A:135:VAL:HG11	1:A:232:VAL:HB	0.58	1.73	1	1
1:A:258:GLN:HA	1:A:261:LEU:HD12	0.58	1.74	1	1
1:A:93:LEU:HD11	1:A:173:GLY:HA2	0.58	1.75	4	1
1:A:135:VAL:HG11	1:A:232:VAL:HG23	0.58	1.74	19	1
1:A:227:ASP:O	1:A:229:LEU:N	0.58	2.37	5	2
1:A:187:GLN:NE2	1:A:190:VAL:HG13	0.58	2.12	7	1
1:A:71:LEU:HD11	1:A:155:LEU:HD21	0.58	1.75	10	3
1:A:71:LEU:HD13	1:A:104:LEU:HD22	0.58	1.75	17	2
1:A:102:ALA:HB3	1:A:252:LEU:CD2	0.58	2.28	9	7
1:A:42:THR:HG22	1:A:221:MET:HG3	0.58	1.75	20	3
1:A:75:LYS:HE3	1:A:97:LEU:HD21	0.58	1.75	3	1
1:A:149:LEU:HD23	1:A:280:VAL:CG1	0.58	2.29	4	2
1:A:140:HIS:NE2	1:A:239:VAL:HG13	0.58	2.13	6	3
1:A:74:TYR:CE1	1:A:159:LEU:HD13	0.58	2.33	11	1
1:A:156:GLN:HA	1:A:159:LEU:HD12	0.58	1.75	20	1
1:A:32:ARG:HB3	1:A:63:LEU:HD22	0.58	1.75	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:99:ALA:CB	1:A:256:ALA:HB2	0.58	2.28	9	12
1:A:10:PRO:O	1:A:11:GLU:C	0.58	2.41	18	1
1:A:139:SER:CB	1:A:229:LEU:HD23	0.57	2.29	8	1
1:A:264:ARG:NE	1:A:268:LEU:HD21	0.57	2.13	3	1
1:A:30:LEU:HD13	1:A:34:TRP:CH2	0.57	2.33	11	2
1:A:81:GLN:C	1:A:82:LEU:HD23	0.57	2.20	18	5
1:A:155:LEU:O	1:A:155:LEU:HD13	0.57	1.99	3	3
1:A:78:LEU:HD22	1:A:159:LEU:CD2	0.57	2.28	20	2
1:A:14:LEU:HD12	1:A:149:LEU:HD21	0.57	1.75	2	1
1:A:75:LYS:HD3	1:A:97:LEU:HD21	0.57	1.77	19	2
1:A:157:LYS:O	1:A:161:VAL:HG23	0.57	1.99	7	1
1:A:71:LEU:HD11	1:A:155:LEU:CD2	0.57	2.30	19	2
1:A:180:ARG:O	1:A:181:LEU:HD22	0.57	2.00	10	3
1:A:71:LEU:HD11	1:A:155:LEU:HD22	0.57	1.77	1	2
1:A:180:ARG:HG3	1:A:181:LEU:HD22	0.57	1.76	16	1
1:A:14:LEU:HD13	1:A:149:LEU:CD1	0.56	2.30	6	1
1:A:40:VAL:O	1:A:42:THR:HG23	0.56	2.00	14	1
1:A:3:GLU:O	1:A:6:VAL:HG22	0.56	2.00	18	1
1:A:60:LEU:HD22	1:A:111:VAL:CG1	0.56	2.30	2	1
1:A:250:ILE:O	1:A:254:ALA:HB2	0.56	2.01	11	5
1:A:82:LEU:HD11	1:A:169:GLY:C	0.56	2.21	17	2
1:A:75:LYS:CE	1:A:159:LEU:HD11	0.56	2.30	9	1
1:A:33:PHE:CE2	1:A:148:LEU:HD22	0.56	2.36	20	2
1:A:181:LEU:HD21	1:A:186:GLU:OE2	0.56	2.01	12	1
1:A:37:LEU:HD12	1:A:145:ARG:HG2	0.56	1.76	15	2
1:A:32:ARG:CD	1:A:63:LEU:HD22	0.56	2.30	15	1
1:A:78:LEU:HD23	1:A:159:LEU:HD22	0.56	1.77	15	1
1:A:210:TRP:CZ2	1:A:214:LEU:HD22	0.56	2.36	7	1
1:A:81:GLN:C	1:A:82:LEU:HD13	0.56	2.20	15	2
1:A:280:VAL:HG13	1:A:281:GLU:CD	0.56	2.21	15	2
1:A:114:ARG:NH1	1:A:137:LEU:HD13	0.56	2.15	19	1
1:A:228:ARG:C	1:A:229:LEU:HD12	0.56	2.20	8	2
1:A:68:MET:CE	1:A:190:VAL:HG11	0.56	2.30	5	1
1:A:40:VAL:HG23	1:A:56:VAL:HG21	0.56	1.78	3	1
1:A:8:THR:HG21	1:A:149:LEU:HD23	0.56	1.75	9	2
1:A:84:PRO:HD3	1:A:164:ALA:HB3	0.56	1.77	16	2
1:A:21:GLN:CG	1:A:160:ALA:HB2	0.56	2.31	17	2
1:A:75:LYS:NZ	1:A:97:LEU:HD22	0.55	2.15	6	2
1:A:39:TRP:NE1	1:A:214:LEU:HD21	0.55	2.16	13	1
1:A:8:THR:HG22	1:A:280:VAL:CG2	0.55	2.31	15	1
1:A:243:LEU:HD21	1:A:293:PRO:HA	0.55	1.78	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:111:VAL:HA	1:A:144:LEU:HD21	0.55	1.78	1	3
1:A:75:LYS:HE2	1:A:159:LEU:HD11	0.55	1.78	9	1
1:A:180:ARG:HG2	1:A:181:LEU:HD23	0.55	1.76	7	1
1:A:18:THR:HG22	1:A:156:GLN:HG3	0.55	1.77	12	3
1:A:29:ALA:HB3	1:A:70:GLU:OE2	0.55	2.01	10	1
1:A:33:PHE:CE2	1:A:148:LEU:HD13	0.55	2.37	20	1
1:A:135:VAL:HG21	1:A:232:VAL:HG23	0.55	1.78	14	4
1:A:187:GLN:CD	1:A:190:VAL:HG13	0.55	2.21	7	1
1:A:103:ARG:NH1	1:A:252:LEU:HD13	0.55	2.17	19	3
1:A:267:PRO:O	1:A:268:LEU:HD23	0.55	2.02	13	2
1:A:248:GLN:OE1	1:A:252:LEU:HD21	0.55	2.00	11	6
1:A:100:ALA:HB1	1:A:155:LEU:HD23	0.55	1.77	7	1
1:A:141:LEU:HD23	1:A:145:ARG:NH2	0.55	2.16	14	1
1:A:103:ARG:HG2	1:A:252:LEU:HD22	0.54	1.76	3	3
1:A:50:GLU:OE2	1:A:56:VAL:HG13	0.54	2.02	4	1
1:A:47:VAL:HG22	1:A:118:TYR:OH	0.54	2.02	19	1
1:A:118:TYR:O	1:A:122:VAL:HG22	0.54	2.01	1	1
1:A:149:LEU:HD23	1:A:280:VAL:HG13	0.54	1.78	7	1
1:A:110:ASP:HB3	1:A:144:LEU:HD13	0.54	1.78	12	3
1:A:75:LYS:HD3	1:A:97:LEU:HD23	0.54	1.77	14	1
1:A:104:LEU:HD11	1:A:108:MET:CE	0.54	2.32	4	4
1:A:83:THR:HG22	1:A:161:VAL:HG11	0.54	1.80	5	1
1:A:18:THR:HG23	1:A:156:GLN:HG3	0.54	1.78	19	1
1:A:60:LEU:HD12	1:A:115:LEU:HD21	0.54	1.79	17	1
1:A:18:THR:HG22	1:A:156:GLN:HG2	0.54	1.77	1	1
1:A:140:HIS:CE1	1:A:239:VAL:HG22	0.54	2.38	18	2
1:A:51:LEU:HD22	1:A:119:ARG:CA	0.54	2.33	15	1
1:A:45:GLU:HA	1:A:130:THR:HG21	0.54	1.78	10	3
1:A:93:LEU:HD23	1:A:94:SER:N	0.54	2.18	18	1
1:A:233:LYS:HB2	1:A:236:VAL:HG22	0.54	1.78	7	3
1:A:155:LEU:HD23	1:A:159:LEU:HD22	0.54	1.80	8	1
1:A:257:ALA:O	1:A:261:LEU:HD13	0.54	2.02	17	2
1:A:140:HIS:NE2	1:A:144:LEU:HD12	0.54	2.17	17	1
1:A:51:LEU:HD22	1:A:122:VAL:HG21	0.54	1.78	16	1
1:A:191:ARG:O	1:A:194:THR:HG22	0.54	2.03	20	6
1:A:140:HIS:NE2	1:A:239:VAL:HG22	0.54	2.18	12	3
1:A:33:PHE:CE1	1:A:148:LEU:HD13	0.54	2.38	12	1
1:A:264:ARG:HH11	1:A:268:LEU:HD21	0.53	1.63	5	4
1:A:39:TRP:CD1	1:A:214:LEU:HD11	0.53	2.37	13	1
1:A:224:ARG:O	1:A:225:THR:HG22	0.53	2.03	14	3
1:A:140:HIS:NE2	1:A:239:VAL:HG23	0.53	2.17	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:144:LEU:HD13	1:A:242:LYS:HE2	0.53	1.80	19	1
1:A:51:LEU:HD21	1:A:118:TYR:CZ	0.53	2.38	16	1
1:A:236:VAL:HG22	1:A:236:VAL:O	0.53	2.04	13	2
1:A:97:LEU:HD22	1:A:177:ILE:HG22	0.53	1.79	11	1
1:A:266:GLU:HB2	1:A:267:PRO:CD	0.53	2.33	6	7
1:A:280:VAL:HG13	1:A:281:GLU:HG3	0.53	1.81	15	3
1:A:51:LEU:CD1	1:A:122:VAL:HG11	0.53	2.33	17	2
1:A:101:GLN:OE1	1:A:177:ILE:HD12	0.53	2.03	13	1
1:A:33:PHE:HA	1:A:63:LEU:HD13	0.53	1.80	8	3
1:A:33:PHE:CE1	1:A:37:LEU:HD23	0.53	2.39	19	1
1:A:139:SER:HB2	1:A:229:LEU:HD22	0.53	1.81	7	2
1:A:33:PHE:CE2	1:A:148:LEU:HD21	0.53	2.39	7	1
1:A:142:ARG:NH2	1:A:229:LEU:HD11	0.53	2.19	13	2
1:A:40:VAL:HG13	1:A:56:VAL:HG11	0.53	1.81	17	1
1:A:133:LEU:HD12	1:A:134:ARG:N	0.53	2.19	17	1
1:A:155:LEU:HD23	1:A:155:LEU:O	0.53	2.03	14	3
1:A:33:PHE:CE2	1:A:60:LEU:HD22	0.53	2.38	3	1
1:A:74:TYR:O	1:A:78:LEU:HD12	0.52	2.04	2	1
1:A:83:THR:HG21	1:A:266:GLU:OE2	0.52	2.03	2	2
1:A:233:LYS:HB3	1:A:236:VAL:HG22	0.52	1.80	6	1
1:A:146:LYS:HG2	1:A:280:VAL:HG21	0.52	1.80	11	1
1:A:290:SER:O	1:A:291:ALA:HB3	0.52	2.04	20	2
1:A:118:TYR:CZ	1:A:122:VAL:HG21	0.52	2.39	20	1
1:A:8:THR:HG21	1:A:149:LEU:HD21	0.52	1.80	12	1
1:A:78:LEU:O	1:A:78:LEU:HD13	0.52	2.05	16	1
1:A:144:LEU:HD12	1:A:242:LYS:HE3	0.52	1.81	5	1
1:A:78:LEU:CD1	1:A:159:LEU:HD22	0.52	2.24	2	1
1:A:93:LEU:HD12	1:A:93:LEU:O	0.52	2.04	17	3
1:A:252:LEU:HD13	1:A:253:GLN:N	0.52	2.20	14	1
1:A:33:PHE:CE2	1:A:148:LEU:HD23	0.52	2.40	1	1
1:A:232:VAL:O	1:A:233:LYS:C	0.52	2.48	15	8
1:A:83:THR:HG21	1:A:266:GLU:CD	0.52	2.24	2	1
1:A:43:LEU:HD21	1:A:226:ARG:HB2	0.52	1.79	8	1
1:A:78:LEU:HD21	1:A:97:LEU:HD11	0.52	1.81	11	1
1:A:279:GLN:O	1:A:280:VAL:HG13	0.52	2.04	17	5
1:A:22:SER:OG	1:A:30:LEU:HD21	0.52	2.03	14	1
1:A:14:LEU:HD12	1:A:14:LEU:O	0.52	2.03	18	1
1:A:114:ARG:CZ	1:A:137:LEU:HD12	0.52	2.34	6	1
1:A:133:LEU:HD23	1:A:234:GLU:O	0.52	2.05	12	1
1:A:93:LEU:HD12	1:A:162:TYR:CZ	0.52	2.39	18	1
1:A:40:VAL:HG13	1:A:141:LEU:HD21	0.52	1.82	19	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:LEU:HD13	1:A:221:MET:HB2	0.52	1.80	13	1
1:A:99:ALA:HB1	1:A:252:LEU:CD2	0.52	2.35	14	1
1:A:97:LEU:HD23	1:A:101:GLN:HG2	0.51	1.80	4	2
1:A:268:LEU:HD12	1:A:270:GLU:HG2	0.51	1.81	5	4
1:A:243:LEU:CD2	1:A:294:VAL:HG22	0.51	2.24	16	1
1:A:90:ARG:NH1	1:A:91:ALA:HB2	0.51	2.21	5	1
1:A:51:LEU:HD22	1:A:119:ARG:HA	0.51	1.82	15	2
1:A:103:ARG:NH1	1:A:252:LEU:HD23	0.51	2.20	8	1
1:A:82:LEU:CB	1:A:93:LEU:HD22	0.51	2.35	20	1
1:A:85:VAL:HG21	1:A:89:THR:HG21	0.51	1.82	15	5
1:A:82:LEU:HD12	1:A:93:LEU:HD22	0.51	1.83	6	1
1:A:82:LEU:CD1	1:A:93:LEU:HD13	0.51	2.35	8	1
1:A:42:THR:HG22	1:A:217:ARG:CD	0.51	2.35	15	2
1:A:11:GLU:HB2	1:A:14:LEU:HD23	0.51	1.83	18	1
1:A:118:TYR:CE2	1:A:122:VAL:HG21	0.51	2.41	20	1
1:A:51:LEU:HD22	1:A:122:VAL:HB	0.51	1.82	2	1
1:A:229:LEU:HB2	1:A:291:ALA:HB3	0.51	1.83	17	2
1:A:60:LEU:HA	1:A:63:LEU:HD12	0.51	1.82	17	2
1:A:110:ASP:CB	1:A:144:LEU:HD13	0.51	2.35	12	1
1:A:146:LYS:HD3	1:A:280:VAL:HG21	0.51	1.82	2	2
1:A:180:ARG:HG3	1:A:181:LEU:HD23	0.51	1.81	2	1
1:A:40:VAL:HG22	1:A:56:VAL:HB	0.51	1.81	13	1
1:A:74:TYR:CE2	1:A:159:LEU:HD11	0.51	2.41	13	1
1:A:57:THR:HG23	1:A:115:LEU:HB2	0.51	1.83	8	3
1:A:43:LEU:HD22	1:A:137:LEU:HD21	0.51	1.83	7	1
1:A:85:VAL:HG11	1:A:89:THR:CG2	0.51	2.36	1	6
1:A:42:THR:O	1:A:43:LEU:HD12	0.51	2.06	13	2
1:A:112:CYS:SG	1:A:193:ALA:HB1	0.50	2.45	14	2
1:A:51:LEU:CD2	1:A:122:VAL:HG11	0.50	2.33	4	1
1:A:228:ARG:C	1:A:229:LEU:HD23	0.50	2.26	16	8
1:A:14:LEU:HD12	1:A:149:LEU:HD11	0.50	1.82	10	1
1:A:102:ALA:CB	1:A:252:LEU:HD21	0.50	2.35	1	1
1:A:47:VAL:O	1:A:51:LEU:HD12	0.50	2.06	2	1
1:A:103:ARG:NH2	1:A:106:ALA:HB3	0.50	2.21	11	2
1:A:118:TYR:O	1:A:122:VAL:HG23	0.50	2.06	11	7
1:A:99:ALA:HB1	1:A:252:LEU:O	0.50	2.07	17	3
1:A:52:LEU:HD12	1:A:52:LEU:O	0.50	2.06	15	2
1:A:280:VAL:HG13	1:A:281:GLU:CG	0.50	2.37	15	1
1:A:214:LEU:HD13	1:A:214:LEU:O	0.50	2.07	6	3
1:A:29:ALA:HB1	1:A:67:THR:OG1	0.50	2.07	12	3
1:A:48:GLN:HB2	1:A:130:THR:HG22	0.50	1.83	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:135:VAL:HG11	1:A:232:VAL:N	0.50	2.22	18	6
1:A:99:ALA:HB3	1:A:256:ALA:HB2	0.50	1.83	19	2
1:A:40:VAL:HG22	1:A:56:VAL:CG1	0.50	2.36	17	1
1:A:29:ALA:HB2	1:A:66:GLU:HG2	0.49	1.83	5	4
1:A:14:LEU:HD22	1:A:149:LEU:CD2	0.49	2.36	6	1
1:A:51:LEU:HD12	1:A:51:LEU:O	0.49	2.07	6	1
1:A:18:THR:HG21	1:A:34:TRP:CH2	0.49	2.42	7	1
1:A:51:LEU:CD1	1:A:122:VAL:HG21	0.49	2.36	7	2
1:A:78:LEU:HD22	1:A:159:LEU:HD13	0.49	1.83	7	1
1:A:210:TRP:NE1	1:A:214:LEU:HD12	0.49	2.20	9	1
1:A:78:LEU:HD11	1:A:163:GLN:HA	0.49	1.84	12	1
1:A:142:ARG:NH2	1:A:229:LEU:HD21	0.49	2.22	19	2
1:A:194:THR:O	1:A:198:LEU:HD12	0.49	2.07	19	1
1:A:43:LEU:HD23	1:A:217:ARG:CG	0.49	2.37	16	2
1:A:75:LYS:HE3	1:A:97:LEU:HD23	0.49	1.84	8	1
1:A:239:VAL:HG13	1:A:243:LEU:HD23	0.49	1.82	8	1
1:A:40:VAL:HG23	1:A:56:VAL:HG11	0.49	1.83	1	1
1:A:82:LEU:HD22	1:A:93:LEU:HD11	0.49	1.83	1	1
1:A:82:LEU:HD12	1:A:169:GLY:C	0.49	2.27	9	1
1:A:43:LEU:HD22	1:A:134:ARG:NH2	0.49	2.22	12	1
1:A:79:GLU:HA	1:A:82:LEU:HD11	0.49	1.83	15	1
1:A:266:GLU:N	1:A:267:PRO:HD2	0.49	2.22	4	20
1:A:9:GLU:CB	1:A:10:PRO:CD	0.49	2.91	18	19
1:A:51:LEU:HD22	1:A:122:VAL:CG1	0.49	2.38	9	2
1:A:99:ALA:O	1:A:252:LEU:HD23	0.49	2.08	1	1
1:A:103:ARG:HH11	1:A:252:LEU:HD13	0.49	1.68	3	1
1:A:82:LEU:HD22	1:A:82:LEU:N	0.49	2.22	15	3
1:A:83:THR:CG2	1:A:161:VAL:HG11	0.49	2.37	8	1
1:A:82:LEU:HD11	1:A:169:GLY:HA3	0.49	1.84	20	2
1:A:135:VAL:HG13	1:A:230:ASP:N	0.49	2.23	18	3
1:A:43:LEU:HD23	1:A:217:ARG:HG2	0.49	1.83	4	1
1:A:85:VAL:HG13	1:A:266:GLU:OE2	0.49	2.07	11	1
1:A:71:LEU:HD23	1:A:104:LEU:HD22	0.49	1.85	14	1
1:A:9:GLU:N	1:A:10:PRO:HD2	0.48	2.23	3	20
1:A:33:PHE:HA	1:A:63:LEU:HD12	0.48	1.83	4	1
1:A:43:LEU:HD11	1:A:225:THR:HB	0.48	1.84	6	1
1:A:71:LEU:HD13	1:A:104:LEU:CD2	0.48	2.37	11	2
1:A:118:TYR:CE2	1:A:137:LEU:HD13	0.48	2.42	16	2
1:A:114:ARG:NH1	1:A:137:LEU:HD12	0.48	2.22	4	1
1:A:8:THR:OG1	1:A:14:LEU:HD21	0.48	2.08	5	1
1:A:224:ARG:O	1:A:225:THR:C	0.48	2.51	7	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:108:MET:SD	1:A:190:VAL:HG11	0.48	2.47	12	1
1:A:128:GLN:HG3	1:A:133:LEU:HD11	0.48	1.82	20	2
1:A:58:GLN:OE1	1:A:198:LEU:HD23	0.48	2.07	5	1
1:A:85:VAL:HG12	1:A:87:GLU:H	0.48	1.68	9	2
1:A:140:HIS:CE1	1:A:144:LEU:HD22	0.48	2.43	8	1
1:A:75:LYS:HE2	1:A:97:LEU:HD11	0.48	1.85	19	1
1:A:135:VAL:HG23	1:A:230:ASP:H	0.48	1.69	1	1
1:A:118:TYR:CE1	1:A:122:VAL:HG21	0.48	2.44	6	1
1:A:210:TRP:HE1	1:A:214:LEU:HD12	0.48	1.68	9	1
1:A:37:LEU:HD11	1:A:145:ARG:CG	0.48	2.39	18	2
1:A:39:TRP:O	1:A:42:THR:HG22	0.48	2.09	16	1
1:A:5:ALA:HB2	1:A:142:ARG:O	0.48	2.08	17	1
1:A:39:TRP:NE1	1:A:214:LEU:HD11	0.48	2.23	1	2
1:A:14:LEU:CD1	1:A:149:LEU:HD21	0.48	2.39	10	3
1:A:8:THR:OG1	1:A:149:LEU:HD21	0.48	2.08	4	2
1:A:21:GLN:HG3	1:A:160:ALA:HB2	0.48	1.84	17	2
1:A:126:LEU:C	1:A:126:LEU:HD13	0.48	2.30	16	1
1:A:82:LEU:HD13	1:A:93:LEU:HD13	0.47	1.86	18	2
1:A:33:PHE:CE1	1:A:60:LEU:HD23	0.47	2.44	10	1
1:A:266:GLU:CB	1:A:267:PRO:CD	0.47	2.93	19	14
1:A:280:VAL:O	1:A:281:GLU:C	0.47	2.53	8	2
1:A:133:LEU:HD23	1:A:235:GLN:HG3	0.47	1.86	1	1
1:A:190:VAL:O	1:A:193:ALA:HB3	0.47	2.10	7	3
1:A:292:ALA:HB1	1:A:293:PRO:HD2	0.47	1.87	1	14
1:A:135:VAL:HG13	1:A:230:ASP:H	0.47	1.69	2	4
1:A:83:THR:HG23	1:A:162:TYR:CD1	0.47	2.44	3	1
1:A:56:VAL:O	1:A:60:LEU:HD12	0.47	2.10	10	1
1:A:196:GLY:O	1:A:199:ALA:HB3	0.47	2.09	15	4
1:A:142:ARG:CZ	1:A:229:LEU:HD21	0.47	2.40	10	1
1:A:149:LEU:HD23	1:A:150:ARG:N	0.47	2.24	10	1
1:A:121:GLU:OE2	1:A:237:ALA:HB3	0.47	2.09	19	1
1:A:37:LEU:HD21	1:A:145:ARG:HG2	0.47	1.87	17	2
1:A:195:VAL:O	1:A:199:ALA:HB2	0.47	2.08	7	1
1:A:43:LEU:HD11	1:A:220:GLU:CG	0.47	2.40	3	1
1:A:14:LEU:CD2	1:A:149:LEU:HD21	0.47	2.40	7	2
1:A:94:SER:HA	1:A:176:ALA:HB2	0.47	1.87	7	2
1:A:89:THR:HG23	1:A:90:ARG:HE	0.47	1.70	15	1
1:A:8:THR:OG1	1:A:14:LEU:HD11	0.47	2.09	5	1
1:A:56:VAL:CG2	1:A:115:LEU:HD11	0.47	2.40	6	2
1:A:243:LEU:HD12	1:A:294:VAL:O	0.47	2.10	8	1
1:A:83:THR:HG23	1:A:85:VAL:HG23	0.47	1.86	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:LEU:C	1:A:37:LEU:HD13	0.46	2.31	2	5
1:A:43:LEU:HD11	1:A:226:ARG:CB	0.46	2.39	8	1
1:A:114:ARG:HH22	1:A:137:LEU:HD12	0.46	1.71	10	3
1:A:37:LEU:O	1:A:37:LEU:HD22	0.46	2.11	2	1
1:A:99:ALA:HB1	1:A:252:LEU:HD22	0.46	1.85	14	1
1:A:33:PHE:CZ	1:A:37:LEU:HD23	0.46	2.45	19	1
1:A:83:THR:HG22	1:A:84:PRO:HD2	0.46	1.87	2	1
1:A:27:GLU:OE2	1:A:30:LEU:HD11	0.46	2.10	8	1
1:A:135:VAL:HG11	1:A:232:VAL:CG2	0.46	2.41	8	1
1:A:231:GLU:CA	1:A:291:ALA:HB2	0.46	2.41	11	1
1:A:155:LEU:O	1:A:159:LEU:HD23	0.46	2.11	18	1
1:A:82:LEU:HG	1:A:166:ALA:HB3	0.46	1.87	20	4
1:A:136:ARG:CD	1:A:239:VAL:HG21	0.46	2.40	1	1
1:A:57:THR:HA	1:A:115:LEU:HD23	0.46	1.86	11	1
1:A:261:LEU:HD12	1:A:272:MET:HG2	0.46	1.88	3	1
1:A:111:VAL:HG22	1:A:144:LEU:CD2	0.46	2.40	11	1
1:A:111:VAL:O	1:A:115:LEU:HD13	0.46	2.11	4	1
1:A:93:LEU:CD2	1:A:97:LEU:HD13	0.46	2.40	5	1
1:A:268:LEU:HD11	1:A:271:ASP:HB2	0.46	1.87	19	1
1:A:231:GLU:H	1:A:291:ALA:HB2	0.46	1.69	10	1
1:A:75:LYS:HD2	1:A:97:LEU:HD11	0.46	1.87	4	1
1:A:149:LEU:CD2	1:A:280:VAL:HG13	0.46	2.41	7	1
1:A:60:LEU:HD13	1:A:111:VAL:HG12	0.46	1.88	12	1
1:A:75:LYS:CD	1:A:177:ILE:HD12	0.46	2.41	17	1
1:A:264:ARG:HE	1:A:268:LEU:HD21	0.45	1.69	3	1
1:A:248:GLN:O	1:A:252:LEU:HD12	0.45	2.11	6	1
1:A:57:THR:HG23	1:A:115:LEU:HB3	0.45	1.88	15	2
1:A:51:LEU:HD13	1:A:122:VAL:CG1	0.45	2.41	17	1
1:A:43:LEU:HD12	1:A:47:VAL:HG23	0.45	1.89	19	1
1:A:136:ARG:HH11	1:A:239:VAL:HG21	0.45	1.70	2	1
1:A:82:LEU:HD13	1:A:93:LEU:HD11	0.45	1.88	16	1
1:A:228:ARG:O	1:A:229:LEU:HD23	0.45	2.11	5	1
1:A:107:ASP:HB3	1:A:148:LEU:HD12	0.45	1.87	8	1
1:A:74:TYR:CE2	1:A:78:LEU:HD11	0.45	2.47	18	1
1:A:43:LEU:HD23	1:A:221:MET:HA	0.45	1.88	3	1
1:A:82:LEU:HB2	1:A:166:ALA:HB3	0.45	1.86	6	1
1:A:144:LEU:HD23	1:A:144:LEU:O	0.45	2.11	6	1
1:A:43:LEU:HD13	1:A:137:LEU:HD23	0.45	1.89	7	1
1:A:40:VAL:O	1:A:41:GLN:C	0.45	2.55	13	1
1:A:112:CYS:HB2	1:A:193:ALA:HB1	0.45	1.89	6	1
1:A:74:TYR:CE1	1:A:159:LEU:HD22	0.45	2.47	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:140:HIS:HE1	1:A:239:VAL:HG13	0.45	1.72	12	1
1:A:71:LEU:HD23	1:A:104:LEU:CD2	0.45	2.41	14	1
1:A:288:GLY:O	1:A:289:THR:HG23	0.45	2.11	16	1
1:A:261:LEU:HD23	1:A:272:MET:HG2	0.45	1.87	1	1
1:A:18:THR:HG23	1:A:156:GLN:NE2	0.45	2.27	3	1
1:A:100:ALA:CB	1:A:155:LEU:HD12	0.45	2.40	12	1
1:A:96:GLU:HG3	1:A:259:ALA:HB3	0.45	1.89	20	1
1:A:117:GLN:OE1	1:A:237:ALA:HB1	0.45	2.11	1	1
1:A:51:LEU:HD11	1:A:118:TYR:OH	0.45	2.11	16	2
1:A:37:LEU:HA	1:A:60:LEU:HD21	0.45	1.89	8	2
1:A:40:VAL:HA	1:A:56:VAL:HG11	0.45	1.88	2	1
1:A:110:ASP:HB3	1:A:144:LEU:HD12	0.45	1.89	9	1
1:A:78:LEU:HD23	1:A:159:LEU:CD2	0.45	2.42	15	1
1:A:59:GLU:O	1:A:63:LEU:HD13	0.45	2.12	16	1
1:A:82:LEU:HD21	1:A:166:ALA:HB3	0.45	1.88	8	1
1:A:228:ARG:O	1:A:229:LEU:C	0.45	2.55	14	7
1:A:268:LEU:HD23	1:A:270:GLU:HG3	0.44	1.87	2	1
1:A:93:LEU:HD21	1:A:97:LEU:HD13	0.44	1.88	5	1
1:A:239:VAL:HG22	1:A:243:LEU:CD1	0.44	2.42	5	1
1:A:128:GLN:CG	1:A:133:LEU:HD11	0.44	2.42	13	1
1:A:78:LEU:HD13	1:A:159:LEU:HG	0.44	1.89	9	1
1:A:78:LEU:HD12	1:A:78:LEU:O	0.44	2.11	11	1
1:A:274:ARG:HH21	1:A:275:GLN:NE2	0.44	2.10	12	1
1:A:132:GLU:CA	1:A:232:VAL:HG11	0.44	2.43	14	1
1:A:18:THR:HG23	1:A:156:GLN:OE1	0.44	2.13	17	1
1:A:243:LEU:CG	1:A:294:VAL:HG23	0.44	2.43	2	1
1:A:93:LEU:O	1:A:93:LEU:HD23	0.44	2.12	8	1
1:A:157:LYS:O	1:A:160:ALA:HB3	0.44	2.12	8	2
1:A:8:THR:HG21	1:A:149:LEU:HD22	0.44	1.89	14	1
1:A:78:LEU:HD11	1:A:162:TYR:HB3	0.44	1.87	14	1
1:A:236:VAL:O	1:A:237:ALA:HB3	0.44	2.13	16	1
1:A:14:LEU:O	1:A:18:THR:HG23	0.44	2.12	20	2
1:A:40:VAL:HG13	1:A:141:LEU:CD2	0.44	2.43	10	2
1:A:11:GLU:CB	1:A:14:LEU:HD23	0.44	2.43	18	1
1:A:56:VAL:HG23	1:A:115:LEU:HD13	0.44	1.89	19	1
1:A:243:LEU:HD21	1:A:294:VAL:CG2	0.44	2.43	2	1
1:A:14:LEU:HD13	1:A:149:LEU:HD21	0.44	1.89	3	1
1:A:39:TRP:HE1	1:A:214:LEU:HD11	0.44	1.72	1	1
1:A:129:SER:O	1:A:130:THR:HG23	0.44	2.12	11	1
1:A:229:LEU:HD12	1:A:229:LEU:O	0.44	2.13	19	1
1:A:75:LYS:HZ3	1:A:97:LEU:HD22	0.44	1.73	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:133:LEU:HD23	1:A:235:GLN:NE2	0.44	2.27	19	1
1:A:137:LEU:O	1:A:137:LEU:HD23	0.44	2.12	9	3
1:A:132:GLU:HA	1:A:232:VAL:HG11	0.44	1.88	14	2
1:A:146:LYS:CG	1:A:280:VAL:HG21	0.44	2.42	11	1
1:A:42:THR:HG21	1:A:47:VAL:HG21	0.44	1.89	13	1
1:A:180:ARG:HD2	1:A:181:LEU:HD23	0.44	1.90	17	1
1:A:33:PHE:CE1	1:A:148:LEU:HD22	0.44	2.48	18	1
1:A:107:ASP:CB	1:A:148:LEU:HD13	0.44	2.43	19	1
1:A:291:ALA:O	1:A:292:ALA:HB3	0.44	2.13	20	1
1:A:41:GLN:O	1:A:42:THR:C	0.43	2.55	12	1
1:A:61:ARG:HH11	1:A:62:ALA:HB2	0.43	1.72	8	2
1:A:82:LEU:HB3	1:A:93:LEU:HD22	0.43	1.90	20	1
1:A:85:VAL:HG12	1:A:87:GLU:HG2	0.43	1.90	5	2
1:A:138:ALA:HB3	1:A:229:LEU:CD2	0.43	2.44	13	2
1:A:57:THR:HG23	1:A:115:LEU:CB	0.43	2.43	12	1
1:A:57:THR:CA	1:A:115:LEU:HD23	0.43	2.43	17	1
1:A:34:TRP:CZ3	1:A:149:LEU:HD13	0.43	2.48	19	1
1:A:89:THR:HG21	1:A:266:GLU:OE1	0.43	2.13	3	2
1:A:75:LYS:CE	1:A:177:ILE:HG22	0.43	2.43	2	1
1:A:243:LEU:HD23	1:A:296:SER:CA	0.43	2.43	19	2
1:A:99:ALA:HB2	1:A:255:GLU:HB2	0.43	1.90	6	1
1:A:214:LEU:HD23	1:A:214:LEU:O	0.43	2.13	9	1
1:A:90:ARG:O	1:A:93:LEU:HD23	0.43	2.13	10	1
1:A:14:LEU:HD11	1:A:34:TRP:CH2	0.43	2.48	20	1
1:A:114:ARG:CD	1:A:115:LEU:HD12	0.43	2.43	4	1
1:A:78:LEU:HD12	1:A:162:TYR:CD2	0.43	2.47	5	1
1:A:155:LEU:HD13	1:A:155:LEU:C	0.43	2.34	17	2
1:A:246:GLN:HE22	1:A:249:GLN:NE2	0.43	2.12	16	1
1:A:14:LEU:CD1	1:A:149:LEU:HD11	0.43	2.42	19	1
1:A:40:VAL:CG1	1:A:141:LEU:HD21	0.43	2.44	7	2
1:A:102:ALA:CB	1:A:252:LEU:HD13	0.43	2.44	7	1
1:A:32:ARG:HB3	1:A:63:LEU:HD11	0.43	1.91	10	1
1:A:107:ASP:O	1:A:144:LEU:HD11	0.43	2.14	1	1
1:A:40:VAL:O	1:A:43:LEU:HD21	0.43	2.14	2	1
1:A:85:VAL:HG21	1:A:266:GLU:OE1	0.43	2.14	7	3
1:A:82:LEU:HD23	1:A:162:TYR:CD2	0.42	2.49	4	1
1:A:100:ALA:CB	1:A:155:LEU:HD23	0.42	2.43	17	2
1:A:224:ARG:O	1:A:225:THR:CG2	0.42	2.67	13	2
1:A:135:VAL:HG23	1:A:230:ASP:N	0.42	2.28	1	1
1:A:122:VAL:HG13	1:A:128:GLN:NE2	0.42	2.28	11	1
1:A:40:VAL:HG23	1:A:56:VAL:CB	0.42	2.41	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:112:CYS:O	1:A:116:VAL:HG12	0.42	2.13	20	1
1:A:243:LEU:HD23	1:A:296:SER:C	0.42	2.34	2	1
1:A:227:ASP:C	1:A:228:ARG:CG	0.42	2.87	5	1
1:A:79:GLU:CD	1:A:174:LEU:HD12	0.42	2.34	12	1
1:A:14:LEU:O	1:A:18:THR:HG22	0.42	2.14	7	1
1:A:29:ALA:HB2	1:A:66:GLU:CG	0.42	2.44	7	1
1:A:75:LYS:CE	1:A:97:LEU:HD21	0.42	2.42	3	1
1:A:51:LEU:HD22	1:A:122:VAL:HG11	0.42	1.90	6	1
1:A:214:LEU:C	1:A:214:LEU:HD13	0.42	2.35	15	2
1:A:29:ALA:HA	1:A:63:LEU:HD12	0.42	1.90	13	1
1:A:141:LEU:HD23	1:A:145:ARG:NH1	0.42	2.30	16	1
1:A:103:ARG:N	1:A:252:LEU:HD22	0.42	2.29	19	1
1:A:139:SER:N	1:A:229:LEU:HD22	0.42	2.29	3	1
1:A:59:GLU:O	1:A:63:LEU:HD12	0.42	2.14	8	1
1:A:3:GLU:OE1	1:A:289:THR:HG23	0.42	2.15	10	1
1:A:43:LEU:CD1	1:A:137:LEU:HD21	0.42	2.36	11	1
1:A:68:MET:HE2	1:A:190:VAL:HG11	0.42	1.91	5	1
1:A:100:ALA:HB1	1:A:155:LEU:HG	0.42	1.92	11	1
1:A:78:LEU:HD11	1:A:162:TYR:HB2	0.42	1.92	20	1
1:A:51:LEU:HD11	1:A:118:TYR:CD2	0.42	2.50	8	1
1:A:33:PHE:CZ	1:A:148:LEU:HD11	0.42	2.50	9	1
1:A:150:ARG:HB3	1:A:280:VAL:HG11	0.42	1.90	3	1
1:A:141:LEU:HD23	1:A:145:ARG:HD3	0.42	1.92	4	1
1:A:106:ALA:HB1	1:A:245:GLU:OE2	0.42	2.14	9	1
1:A:33:PHE:CB	1:A:63:LEU:HD11	0.42	2.42	12	1
1:A:82:LEU:CD1	1:A:93:LEU:HD22	0.41	2.44	4	2
1:A:71:LEU:CD1	1:A:104:LEU:HD22	0.41	2.44	17	1
1:A:177:ILE:HD11	1:A:180:ARG:NH2	0.41	2.29	20	1
1:A:249:GLN:HA	1:A:252:LEU:HD12	0.41	1.92	3	1
1:A:41:GLN:NE2	1:A:134:ARG:HH12	0.41	2.13	3	1
1:A:78:LEU:CD2	1:A:159:LEU:HD13	0.41	2.45	7	1
1:A:8:THR:OG1	1:A:14:LEU:HD23	0.41	2.15	12	1
1:A:83:THR:HG22	1:A:93:LEU:CD2	0.41	2.45	16	1
1:A:136:ARG:NH1	1:A:239:VAL:HG21	0.41	2.29	17	1
1:A:229:LEU:HD12	1:A:291:ALA:H	0.41	1.76	5	1
1:A:227:ASP:O	1:A:228:ARG:C	0.41	2.58	14	2
1:A:228:ARG:O	1:A:229:LEU:CB	0.41	2.68	19	1
1:A:14:LEU:HD12	1:A:15:ARG:N	0.41	2.31	8	2
1:A:40:VAL:CG1	1:A:141:LEU:HD11	0.41	2.45	8	1
1:A:78:LEU:HD11	1:A:162:TYR:CB	0.41	2.46	16	1
1:A:130:THR:HA	1:A:133:LEU:HD12	0.41	1.91	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:210:TRP:CH2	1:A:214:LEU:HD22	0.41	2.50	7	1
1:A:30:LEU:HD12	1:A:31:GLY:N	0.41	2.29	11	1
1:A:42:THR:HG22	1:A:221:MET:SD	0.41	2.55	11	1
1:A:14:LEU:HD13	1:A:149:LEU:HG	0.41	1.92	15	1
1:A:14:LEU:HD13	1:A:149:LEU:HD13	0.41	1.91	6	1
1:A:83:THR:HG22	1:A:93:LEU:HD22	0.41	1.93	16	1
1:A:14:LEU:HD11	1:A:34:TRP:HH2	0.41	1.76	20	1
1:A:48:GLN:CB	1:A:130:THR:HG22	0.41	2.45	4	1
1:A:78:LEU:HD13	1:A:78:LEU:C	0.41	2.36	14	1
1:A:136:ARG:HD2	1:A:239:VAL:HG21	0.41	1.92	8	2
1:A:69:LYS:O	1:A:73:ALA:HB2	0.41	2.15	4	2
1:A:37:LEU:HD13	1:A:37:LEU:C	0.41	2.36	6	2
1:A:149:LEU:CD2	1:A:280:VAL:HG22	0.41	2.46	6	1
1:A:233:LYS:O	1:A:235:GLN:N	0.41	2.54	6	1
1:A:90:ARG:CA	1:A:93:LEU:HD23	0.41	2.42	7	1
1:A:64:MET:CE	1:A:190:VAL:HG13	0.41	2.46	8	1
1:A:209:ALA:HB3	1:A:213:ARG:HG3	0.41	1.92	14	1
1:A:181:LEU:HD22	1:A:186:GLU:H	0.41	1.76	20	1
1:A:83:THR:HG23	1:A:161:VAL:HG11	0.41	1.93	8	1
1:A:129:SER:O	1:A:133:LEU:HD12	0.41	2.15	8	1
1:A:228:ARG:O	1:A:229:LEU:HD12	0.41	2.15	8	1
1:A:71:LEU:CD2	1:A:104:LEU:HD23	0.41	2.34	11	1
1:A:126:LEU:HD13	1:A:126:LEU:O	0.41	2.15	16	1
1:A:265:PHE:HA	1:A:269:ALA:HB2	0.41	1.93	20	1
1:A:243:LEU:CD2	1:A:294:VAL:HG23	0.40	2.46	2	1
1:A:68:MET:HG3	1:A:104:LEU:HD21	0.40	1.92	3	1
1:A:135:VAL:HG21	1:A:232:VAL:CB	0.40	2.46	3	1
1:A:100:ALA:HB3	1:A:155:LEU:HD23	0.40	1.92	17	1
1:A:266:GLU:N	1:A:267:PRO:CD	0.40	2.85	4	1
1:A:75:LYS:HE2	1:A:97:LEU:HD21	0.40	1.94	5	1
1:A:48:GLN:HA	1:A:51:LEU:HD12	0.40	1.93	7	1
1:A:14:LEU:HD13	1:A:149:LEU:CD2	0.40	2.46	3	1
1:A:239:VAL:HG22	1:A:243:LEU:HD22	0.40	1.93	17	1
1:A:132:GLU:O	1:A:135:VAL:HG12	0.40	2.17	1	1
1:A:232:VAL:O	1:A:232:VAL:HG12	0.40	2.17	15	1
1:A:280:VAL:O	1:A:281:GLU:CB	0.40	2.68	18	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	277/307 (90%)	216±5 (78±2%)	46±6 (17±2%)	15±2 (6±1%)	3	23
All	All	5540/6140 (90%)	4310 (78%)	923 (17%)	307 (6%)	3	23

All 43 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	24	GLN	20
1	A	224	ARG	20
1	A	269	ALA	20
1	A	280	VAL	19
1	A	227	ASP	17
1	A	164	ALA	15
1	A	229	LEU	15
1	A	225	THR	13
1	A	237	ALA	11
1	A	85	VAL	10
1	A	188	GLY	10
1	A	281	GLU	10
1	A	44	SER	10
1	A	231	GLU	10
1	A	232	VAL	8
1	A	42	THR	8
1	A	43	LEU	7
1	A	233	LYS	7
1	A	87	GLU	6
1	A	189	ARG	6
1	A	41	GLN	6
1	A	88	GLU	6
1	A	296	SER	5
1	A	3	GLU	5
1	A	129	SER	5
1	A	186	GLU	4
1	A	236	VAL	4

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Mol	Chain	Res	Type	Models (Total)
1	A	127	GLY	3
1	A	128	GLN	3
1	A	130	THR	3
1	A	289	THR	3
1	A	226	ARG	3
1	A	228	ARG	2
1	A	278	GLY	2
1	A	290	SER	2
1	A	86	ALA	2
1	A	288	GLY	1
1	A	234	GLU	1
1	A	287	GLU	1
1	A	181	LEU	1
1	A	235	GLN	1
1	A	126	LEU	1
1	A	291	ALA	1

6.3.2　Protein sidechains　ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	227/253 (90%)	160±7 (71±3%)	67±7 (29±3%)	1	17
All	All	4540/5060 (90%)	3207 (71%)	1333 (29%)	1	17

All 189 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	92	ARG	20
1	A	103	ARG	19
1	A	147	ARG	19
1	A	213	ARG	19
1	A	57	THR	18
1	A	90	ARG	17
1	A	235	GLN	17
1	A	274	ARG	17
1	A	229	LEU	17

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Mol	Chain	Res	Type	Models (Total)
1	A	224	ARG	16
1	A	233	LYS	16
1	A	245	GLU	16
1	A	58	GLN	16
1	A	21	GLN	15
1	A	281	GLU	15
1	A	242	LYS	15
1	A	275	GLN	15
1	A	143	LYS	14
1	A	175	SER	14
1	A	114	ARG	14
1	A	134	ARG	13
1	A	227	ASP	13
1	A	43	LEU	13
1	A	93	LEU	13
1	A	97	LEU	13
1	A	158	ARG	13
1	A	226	ARG	13
1	A	9	GLU	12
1	A	39	TRP	12
1	A	53	SER	12
1	A	65	ASP	12
1	A	88	GLU	12
1	A	128	GLN	12
1	A	129	SER	12
1	A	136	ARG	12
1	A	273	GLN	12
1	A	24	GLN	12
1	A	51	LEU	12
1	A	69	LYS	12
1	A	117	GLN	12
1	A	94	SER	12
1	A	260	ARG	12
1	A	220	GLU	11
1	A	25	ARG	11
1	A	261	LEU	11
1	A	148	LEU	11
1	A	54	SER	10
1	A	156	GLN	10
1	A	168	GLU	10
1	A	253	GLN	10
1	A	72	LYS	10

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Mol	Chain	Res	Type	Models (Total)
1	A	142	ARG	10
1	A	181	LEU	10
1	A	61	ARG	9
1	A	78	LEU	9
1	A	83	THR	9
1	A	119	ARG	9
1	A	146	LYS	9
1	A	215	ARG	9
1	A	266	GLU	9
1	A	290	SER	9
1	A	98	GLN	9
1	A	126	LEU	9
1	A	221	MET	9
1	A	249	GLN	9
1	A	289	THR	9
1	A	3	GLU	8
1	A	7	GLU	8
1	A	68	MET	8
1	A	75	LYS	8
1	A	139	SER	8
1	A	225	THR	8
1	A	32	ARG	8
1	A	219	GLU	8
1	A	248	GLN	8
1	A	174	LEU	8
1	A	238	GLU	8
1	A	251	ARG	8
1	A	45	GLU	7
1	A	110	ASP	7
1	A	150	ARG	7
1	A	186	GLU	7
1	A	191	ARG	7
1	A	223	SER	7
1	A	272	MET	7
1	A	123	GLN	7
1	A	153	ASP	7
1	A	262	LYS	7
1	A	44	SER	7
1	A	38	ARG	7
1	A	276	TRP	7
1	A	280	VAL	7
1	A	17	GLN	7

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Mol	Chain	Res	Type	Models (Total)
1	A	48	GLN	7
1	A	13	GLU	6
1	A	4	GLN	6
1	A	133	LEU	6
1	A	163	GLN	6
1	A	180	ARG	6
1	A	214	LEU	6
1	A	258	GLN	6
1	A	35	ASP	6
1	A	279	GLN	6
1	A	82	LEU	6
1	A	42	THR	5
1	A	212	GLU	5
1	A	27	GLU	5
1	A	125	MET	5
1	A	52	LEU	5
1	A	66	GLU	5
1	A	96	GLU	5
1	A	178	ARG	5
1	A	137	LEU	5
1	A	154	ASP	4
1	A	264	ARG	4
1	A	67	THR	4
1	A	118	TYR	4
1	A	217	ARG	4
1	A	230	ASP	4
1	A	36	TYR	4
1	A	41	GLN	4
1	A	50	GLU	4
1	A	85	VAL	4
1	A	87	GLU	4
1	A	159	LEU	4
1	A	37	LEU	4
1	A	187	GLN	4
1	A	198	LEU	4
1	A	76	SER	4
1	A	162	TYR	4
1	A	243	LEU	4
1	A	197	SER	4
1	A	218	MET	4
1	A	81	GLN	3
1	A	172	ARG	3

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Mol	Chain	Res	Type	Models (Total)
1	A	194	THR	3
1	A	252	LEU	3
1	A	109	GLU	3
1	A	231	GLU	3
1	A	19	GLU	3
1	A	228	ARG	3
1	A	240	ARG	3
1	A	157	LYS	3
1	A	130	THR	3
1	A	177	ILE	3
1	A	189	ARG	3
1	A	296	SER	3
1	A	80	GLU	3
1	A	108	MET	3
1	A	132	GLU	2
1	A	263	SER	2
1	A	268	LEU	2
1	A	270	GLU	2
1	A	20	TRP	2
1	A	107	ASP	2
1	A	121	GLU	2
1	A	46	GLN	2
1	A	255	GLU	2
1	A	15	ARG	2
1	A	55	GLN	2
1	A	64	MET	2
1	A	74	TYR	2
1	A	155	LEU	2
1	A	244	GLU	2
1	A	40	VAL	2
1	A	71	LEU	2
1	A	77	GLU	2
1	A	167	ARG	2
1	A	144	LEU	2
1	A	33	PHE	2
1	A	141	LEU	1
1	A	95	LYS	1
1	A	112	CYS	1
1	A	59	GLU	1
1	A	70	GLU	1
1	A	79	GLU	1
1	A	149	LEU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	287	GLU	1
1	A	265	PHE	1
1	A	179	GLU	1
1	A	151	ASP	1
1	A	101	GLN	1
1	A	236	VAL	1
1	A	22	SER	1
1	A	8	THR	1
1	A	11	GLU	1
1	A	14	LEU	1
1	A	171	GLU	1
1	A	210	TRP	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation ⓘ

The completeness of assignment taking into account all chemical shift lists is 67% for the well-defined parts and 67% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_ chem_ shift_ list_ 1*

7.1.1 Bookkeeping ⓘ

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	2810
Number of shifts mapped to atoms	2810
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_\alpha$	298	0.27 ± 0.09	None needed (< 0.5 ppm)
$^{13}C_\beta$	281	0.79 ± 0.04	Should be checked
$^{13}C'$	0	—	None (insufficient data)
^{15}N	289	-1.12 ± 0.13	Should be applied

7.1.3 Completeness of resonance assignments ⓘ

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 67%, i.e. 2617 atoms were assigned a chemical shift out of a possible 3914. 0 out of 51 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	1094/1389 (79%)	546/564 (97%)	277/554 (50%)	271/271 (100%)
Sidechain	1523/2390 (64%)	917/1532 (60%)	606/718 (84%)	0/140 (0%)

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	Total	**¹H**	**¹³C**	**¹⁵N**
Aromatic	0/135 (0%)	0/66 (0%)	0/62 (0%)	0/7 (0%)
Overall	2617/3914 (67%)	1463/2162 (68%)	883/1334 (66%)	271/418 (65%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 67%, i.e. 2810 atoms were assigned a chemical shift out of a possible 4219. 0 out of 56 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	**¹H**	**¹³C**	**¹⁵N**
Backbone	1171/1496 (78%)	584/607 (96%)	298/598 (50%)	289/291 (99%)
Sidechain	1639/2581 (64%)	987/1655 (60%)	652/776 (84%)	0/150 (0%)
Aromatic	0/142 (0%)	0/70 (0%)	0/64 (0%)	0/8 (0%)
Overall	2810/4219 (67%)	1571/2332 (67%)	950/1438 (66%)	289/449 (64%)

7.1.4 Statistically unusual chemical shifts ⓘ

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots ⓘ

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A: